



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2021 – 05:47 PM JST

PDB ID : 6KYB
Title : Crystal structure of Atg18 from *Saccharomyces cerevisiae*
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Deposited on : 2019-09-17
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.18
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

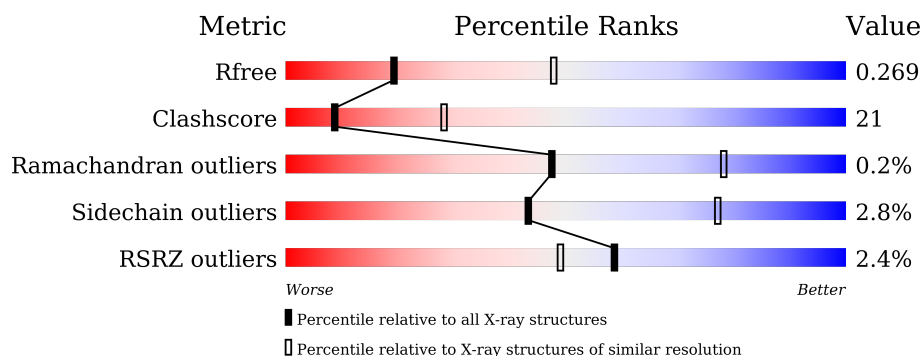
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	<div> <div>45%</div> <div>19%</div> <div>.</div> <div>35%</div> </div>
1	B	505	<div> <div>51%</div> <div>13%</div> <div>.</div> <div>35%</div> </div>
1	C	505	<div> <div>2%</div> <div>35%</div> <div>27%</div> <div>.</div> <div>35%</div> </div>
1	D	505	<div> <div>3%</div> <div>32%</div> <div>28%</div> <div>.</div> <div>37%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9871 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Autophagy-related protein 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2557	1637	418	485	17			
1	B	330	Total	C	N	O	S	0	0	0
			2567	1644	421	486	16			
1	C	328	Total	C	N	O	S	0	0	0
			2517	1612	406	481	18			
1	D	317	Total	C	N	O	S	0	0	0
			2226	1418	359	433	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P43601
A	-3	ALA	-	expression tag	UNP P43601
A	-2	MET	-	expression tag	UNP P43601
A	-1	GLY	-	expression tag	UNP P43601
A	0	SER	-	expression tag	UNP P43601
B	-4	GLY	-	expression tag	UNP P43601
B	-3	ALA	-	expression tag	UNP P43601
B	-2	MET	-	expression tag	UNP P43601
B	-1	GLY	-	expression tag	UNP P43601
B	0	SER	-	expression tag	UNP P43601
C	-4	GLY	-	expression tag	UNP P43601
C	-3	ALA	-	expression tag	UNP P43601
C	-2	MET	-	expression tag	UNP P43601
C	-1	GLY	-	expression tag	UNP P43601
C	0	SER	-	expression tag	UNP P43601
D	-4	GLY	-	expression tag	UNP P43601
D	-3	ALA	-	expression tag	UNP P43601
D	-2	MET	-	expression tag	UNP P43601
D	-1	GLY	-	expression tag	UNP P43601
D	0	SER	-	expression tag	UNP P43601

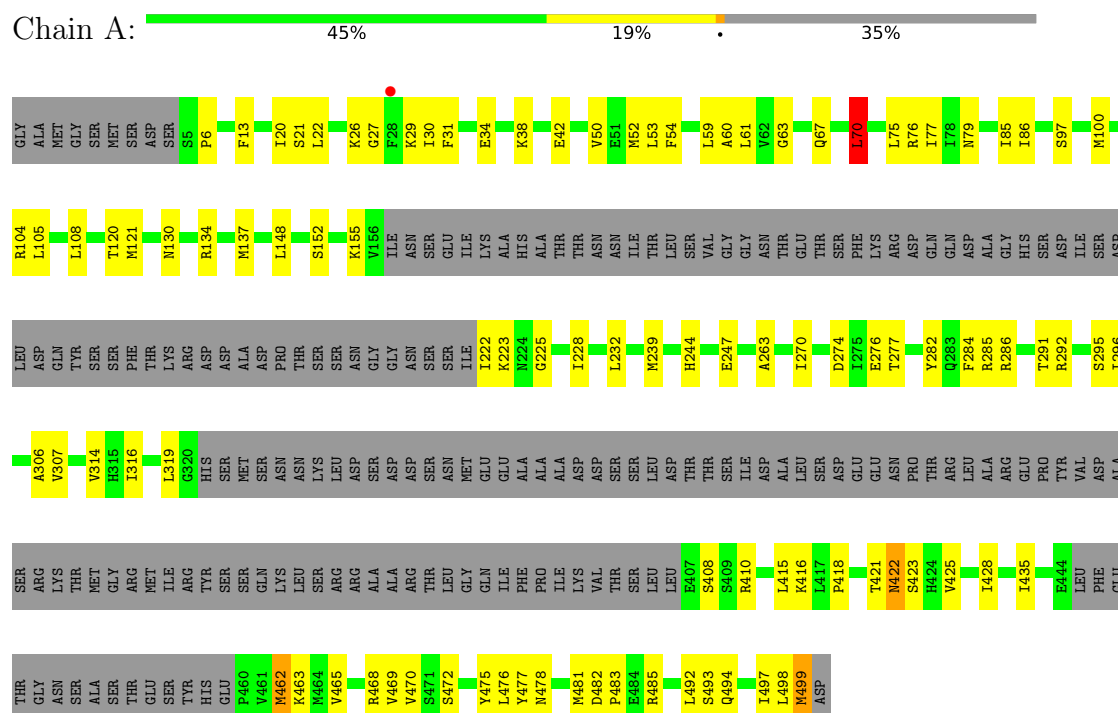
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	O 1	0	0
2	B	3	Total 3	O 3	0	0

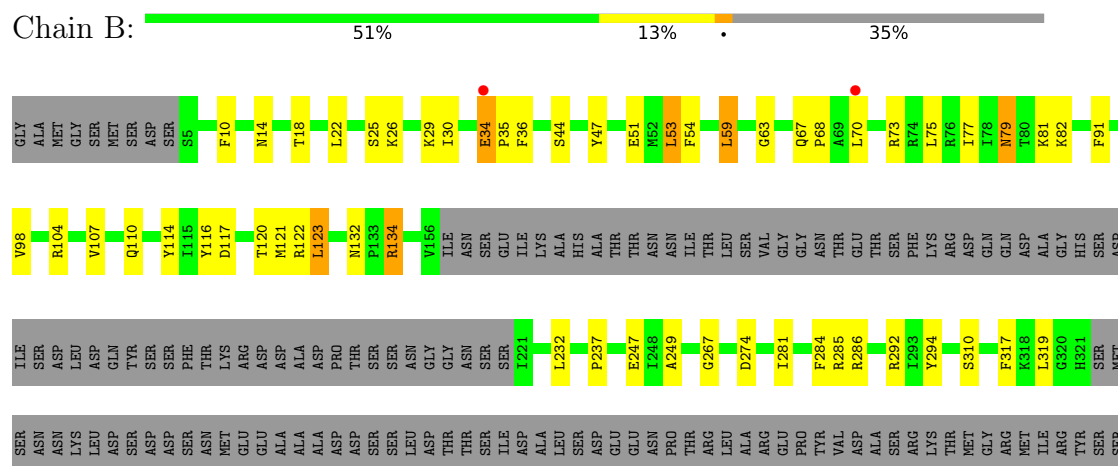
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

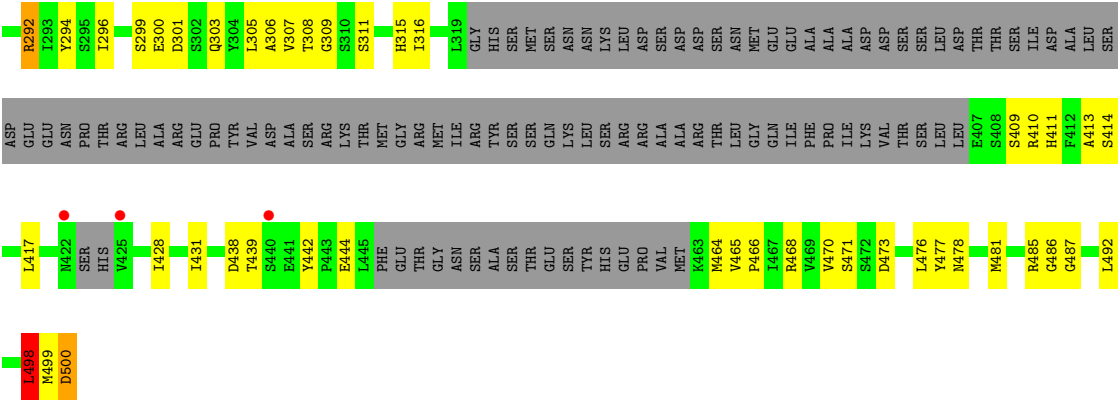
• Molecule 1: Autophagy-related protein 18



• Molecule 1: Autophagy-related protein 18







4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	95.33Å 95.33Å 300.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.63 – 2.80 48.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.63-2.80) 98.4 (48.63-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.214 , 0.267 0.215 , 0.269	Depositor DCC
R_{free} test set	1873 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9871	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2607	0.66	1/3528 (0.0%)
1	B	0.37	0/2618	0.69	5/3544 (0.1%)
1	C	0.41	0/2565	0.84	11/3474 (0.3%)
1	D	0.34	0/2262	0.74	3/3081 (0.1%)
All	All	0.36	0/10052	0.74	20/13627 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	LEU	CB-CG-CD1	8.73	125.84	111.00
1	B	134	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	B	134	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	D	123	LEU	CA-CB-CG	7.28	132.05	115.30
1	C	29	LYS	CA-CB-CG	7.22	129.28	113.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	53	LEU	Peptide
1	B	34	GLU	Peptide
1	B	53	LEU	Peptide
1	C	122	ARG	Peptide
1	C	53	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2557	0	2588	73	0
1	B	2567	0	2597	59	0
1	C	2517	0	2516	124	0
1	D	2226	0	2004	149	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
All	All	9871	0	9705	402	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 402 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ILE:HD11	1:C:498:LEU:HD11	1.30	1.12
1:C:34:GLU:OE2	1:C:478:ASN:ND2	1.90	1.05
1:C:6:PRO:HG2	1:C:498:LEU:HD22	1.41	1.02
1:C:437:ILE:O	1:C:462:MET:HB3	1.63	0.97
1:C:8:ILE:CD1	1:C:498:LEU:HD11	1.94	0.97

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/505 (64%)	302 (94%)	19 (6%)	0	100	100
1	B	322/505 (64%)	305 (95%)	17 (5%)	0	100	100
1	C	320/505 (63%)	288 (90%)	32 (10%)	0	100	100
1	D	305/505 (60%)	229 (75%)	73 (24%)	3 (1%)	15	44
All	All	1268/2020 (63%)	1124 (89%)	141 (11%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	125	HIS
1	D	247	GLU
1	D	64	ILE

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/446 (66%)	288 (98%)	6 (2%)	55	84
1	B	295/446 (66%)	291 (99%)	4 (1%)	67	90
1	C	285/446 (64%)	276 (97%)	9 (3%)	39	73
1	D	215/446 (48%)	203 (94%)	12 (6%)	21	51
All	All	1089/1784 (61%)	1058 (97%)	31 (3%)	43	77

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	285	ARG
1	D	442	TYR
1	C	472	SER
1	D	499	MET
1	D	139	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	283	GLN
1	D	12	ASN
1	D	411	HIS
1	D	79	ASN
1	B	145	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/505 (65%)	-0.12	1 (0%) 94 93	57, 86, 137, 174	0
1	B	330/505 (65%)	-0.29	2 (0%) 89 86	47, 70, 119, 167	0
1	C	328/505 (64%)	-0.03	12 (3%) 41 31	66, 112, 159, 204	0
1	D	317/505 (62%)	0.11	16 (5%) 28 19	68, 137, 193, 221	0
All	All	1304/2020 (64%)	-0.09	31 (2%) 59 49	47, 97, 169, 221	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	TYR	5.3
1	D	138	ALA	4.1
1	D	61	LEU	3.7
1	C	2	SER	3.5
1	D	263	ALA	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.